

# On the analytical formulas for three three-particle integrals with spherical Bessel and Neumann functions.

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(Dated: April 1, 2014)

## Abstract

We derive closed, analytical formulas for the three-particles integrals which include spherical Bessel functions of the first and second kind, i.e., the  $j_\ell(Vr)$  and  $n_\ell(Vr)$  functions. Applications of these formulas to actual calculations of the probabilities of different processes is discussed.

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## I. INTRODUCTION

In our earlier paper [1] we derived formulas for calculations of some three-particles integrals which include spherical Bessel functions  $j_\ell(Vr)$ , where  $\ell = 0, 1, 2$ , which are also called the spherical Bessel functions of the first kind. Generalization of these formulas to higher values of  $\ell$  is possible, but numerical results obtained with the use of these formulas quickly become numerically unstable when  $\ell$  increases and in those cases when  $V \geq 1$ . Moreover, some actual three-body problems require analytical and numerical computations of the three-particles integrals with the spherical Neumann functions  $n_\ell(Vr)$ , where  $\ell$  is integer, which are singular at  $r = 0$ . In some books about Bessel functions (see, e.g., [2]) the functions  $n_\ell(Vr)$  are called the spherical Bessel functions of the 2nd kind. Such problems include various processes of photodetachment and scattering in many three-body systems known from the nuclear, atomic and molecular physics. The goal of this study is to develop an alternative approach which can be used to produce analytical formulas for the three-particle integrals in relative coordinates which include the spherical Bessel functions of the first and second kinds, i.e. the  $j_\ell(Vr)$  and  $n_\ell(Vr)$  functions.

Let us remind that in its most general form the three-particle (or three-body) integral (in relative coordinates) is written in the form

$$I(\alpha, \beta, \gamma; F) = \int_0^{+\infty} \int_0^{+\infty} \int_{|r_{32}-r_{31}|}^{r_{32}+r_{31}} F(r_{32}, r_{31}, r_{21}) \exp(-\alpha r_{32} - \beta r_{31} - \gamma r_{21}) \times \\ r_{32} r_{31} r_{21} dr_{32} dr_{31} dr_{21} \quad (1)$$

where  $\alpha, \beta$  and  $\gamma$  are the three real values which are usually called and considered as the non-linear parameters. The function  $F(r_{32}, r_{31}, r_{21})$  in Eq.(1) is assumed to be a continuous function of all its three variables. In Eq.(1) the three variables  $r_{32}, r_{31}$  and  $r_{21}$  are the three scalar interparticle distances  $r_{ij} = |\mathbf{r}_i - \mathbf{r}_j| = r_{ji}$ , which correspond to the sides (or ribs) of the triangle formed by the three ‘particles’. Note that the three relative coordinates are not completely independent of each other, since, e.g.,  $r_{21} \leq r_{32} + r_{31}$  and  $r_{21} \geq |r_{32} - r_{31}|$ . It complicates analytical and numerical computations of the three-body integrals in the relative coordinates. To avoid this problem in our earlier work we have used three perimetric coordinates  $u_1, u_2, u_3$  which can be expressed as linear combinations of the three relative coordinates  $r_{32}, r_{31}$  and  $r_{21}$  (see, e.g., [1]). The three perimetric coordinates  $u_1, u_2, u_3$  are independent of each other and each of them changes between 0 and  $+\infty$ . This approach is

very general and quickly leads to the final goal, i.e. to the close analytical expressions for the integrals Eq.(1) with different functions  $F(r_{32}, r_{31}, r_{21})$  of three variables  $r_{32}, r_{31}$  and  $r_{21}$ . However, for some functions  $F(r_{32}, r_{31}, r_{21})$  this approach produces very complex expressions which include non-reducible three-dimensional integrals. In such cases it is very difficult and even impossible to finish the process of integration in the perimetric coordinates and obtain the closed expressions for the final formulas.

In this study we apply another approach which is based on the direct integration in the relative coordinates. This approach is not universal and can be applied only in those cases when the function  $F(r_{32}, r_{31}, r_{21})$  depends upon one relative coordinate only. Below, without loss of generality, we shall assume that  $F(r_{32}, r_{31}, r_{21}) = f(r_{32})$ . In this case the three-particle integral, Eq.(1), is written in the form

$$I(\alpha, \beta, \gamma; f) = \int_0^{+\infty} \int_0^{+\infty} \int_{|r_{32}-r_{31}|}^{r_{32}+r_{31}} f(r_{32}) \exp(-\alpha r_{32} - \beta r_{31} - \gamma r_{21}) r_{32} r_{31} r_{21} dr_{32} dr_{31} dr_{21} \quad (2)$$

or, we can write:

$$I(\alpha, \beta, \gamma; f) = -\frac{\partial^3}{\partial \alpha \partial \beta \partial \gamma} J(\alpha, \beta, \gamma; f) \quad (3)$$

where

$$J(\alpha, \beta, \gamma; f) = \int_0^{+\infty} \int_0^{+\infty} \int_{|r_{32}-r_{31}|}^{r_{32}+r_{31}} f(r_{32}) \exp(-\alpha r_{32} - \beta r_{31} - \gamma r_{21}) dr_{32} dr_{31} dr_{21} \quad (4)$$

Our approach developed in this study is based on the following analytical formula for the integral  $J(\alpha, \beta, \gamma; f)$

$$J(\alpha, \beta, \gamma; f) = \frac{2}{\beta^2 - \gamma^2} \left\{ \int_0^{+\infty} f(r_{32}) \exp[-(\alpha + \beta)r_{32}] dr_{32} - \int_0^{+\infty} f(r_{32}) \exp[-(\alpha + \gamma)r_{32}] dr_{32} \right\} \quad (5)$$

where it is additionally assumed that  $\beta \neq \gamma$ . Formally, we can say that the analytical computation of the  $J(\alpha, \beta, \gamma; f)$  integral, Eq.(4), is reduced to the computations of the two Laplace transformations of the function  $f(x)$ . For the first time, I derived this formula in the middle of 1980's. Since then this formula was used in a number of applications, e.g., to derive analytical expressions for the matrix elements of some short-range potentials. It should be mentioned here that any direct application of the formula Eq.(5) is quite restricted, since the backward transition from Eq.(4) to Eq.(2) lead to numerical instabilities in the formulas

arising in this approach for matrix elements. The source of such instabilities is clear, since the integral  $J(\alpha, \beta, \gamma; f)$  takes the form  $\frac{0}{0}$ , when  $\beta \rightarrow \gamma$ . A substantial formula for the  $\frac{0}{0}$  fraction can be obtained with the use of *L'Hôpital's rule*, but then we need to calculate the partial derivatives of the third order from the arising expression. In the next Section we derive the explicit formulas for the integrals  $J(\alpha, \beta, \gamma; f)$  which include the spherical Bessel and Neumann functions. Analytical computations of the derivatives of these formulas is considered in Section III.

## II. FORMULAS FOR THE $J(\alpha, \beta, \gamma; f)$ INTEGRALS

Let us present the explicit formulas for the integrals  $J(\alpha, \beta, \gamma; f)$  which include the spherical Bessel and Neumann functions. First, consider the case of the spherical Bessel functions which are traditionally defined by the equation

$$j_\ell(x) = \sqrt{\frac{2}{\pi x}} J_{\ell+\frac{1}{2}}(x) = \sqrt{\frac{2}{\pi}} x^{\frac{1}{2}-1} J_{\ell+\frac{1}{2}}(x) \quad (6)$$

Therefore, the integral  $J(\alpha, \beta, \gamma; f)$  is written in the form

$$\begin{aligned} J(\alpha, \beta, \gamma; j_\ell(Vr_{32})) &= \sqrt{\frac{2}{\pi}} \int_0^{+\infty} \int_0^{+\infty} \int_{|r_{32}-r_{31}|}^{r_{32}+r_{31}} r_{32}^{\frac{1}{2}-1} J_{\ell+\frac{1}{2}}(Vr_{32}) \exp(-\alpha r_{32} - \beta r_{31} - \gamma r_{21}) \\ dr_{32} dr_{31} dr_{21} &= \sqrt{\frac{2}{\pi}} \frac{2}{\beta^2 - \gamma^2} \left\{ \int_0^{+\infty} r_{32}^{\frac{1}{2}-1} J_{\ell+\frac{1}{2}}(Vr_{32}) \exp[-(\alpha + \beta)r_{32}] dr_{32} \right. \\ &\quad \left. - \int_0^{+\infty} r_{32}^{\frac{1}{2}-1} J_{\ell+\frac{1}{2}}(Vr_{32}) \exp[-(\alpha + \gamma)r_{32}] dr_{32} \right\} \\ &= \sqrt{\frac{2}{\pi}} \frac{2}{\beta^2 - \gamma^2} [F(\alpha + \beta, V) - F(\alpha + \gamma, V)] \end{aligned} \quad (7)$$

where

$$F(\alpha + \beta, V) = \int_0^{+\infty} r_{32}^{\frac{1}{2}-1} \cdot J_{\ell+\frac{1}{2}}(Vr_{32}) \cdot \exp[-(\alpha + \beta)r_{32}] dr_{32} \quad (8)$$

By using the formula Eq.(6.621) from [3] we transform the explicit expression for the  $F(\alpha + \beta, V)$  function to the form

$$F(\alpha + \beta, V) = \frac{\left(\frac{V}{2}\right)^{\ell+\frac{1}{2}}}{[(\alpha + \beta)^2 + V^2]^{\frac{\ell+1}{2}}} \cdot \frac{\ell!}{\Gamma(\ell + \frac{3}{2})} \cdot {}_2F_1\left(\frac{\ell+1}{2}, \frac{\ell+1}{2}; \ell + \frac{3}{2}; q^2\right) \quad (9)$$

where  $q = \frac{V}{\sqrt{(\alpha+\beta)^2 + V^2}} (\leq 1)$  and  $\Gamma(z)$  is the Euler's  $\Gamma$ -function [4]. Note that the hypergeometric function in Eq.(9) is written in the form  ${}_2F_1(a, a; a + a + \frac{1}{2}; y)$ . Therefore, with the

use of the so-called quadratic transformation we can reduce this hypergeometric function to the associated Legendre function of the first kind  $P_\nu^\mu(x)$ . The final expression for the  $F(\alpha + \beta, V)$  function takes the form

$$F(\alpha + \beta, V) = \frac{\ell!}{[(\alpha + \beta)^2 + V^2]^{\frac{1}{4}}} \cdot P_{-\frac{1}{2}}^{-\ell-\frac{1}{2}}\left(\frac{\alpha + \beta}{\sqrt{[(\alpha + \beta)^2 + V^2]}}\right) \quad (10)$$

Analogous formulas can be produced for the spherical Bessel functions of the second kind (or Neumann functions) which are defined by the equation

$$n_\ell(x) = \sqrt{\frac{2}{\pi x}} N_{\ell+\frac{1}{2}}(x) = \sqrt{\frac{2}{\pi}} x^{\frac{1}{2}-1} N_{\ell+\frac{1}{2}}(x) \quad (11)$$

The corresponding three-body integral  $I(\alpha, \beta, \gamma; n_\ell(Vr_{32}))$  is written in the form

$$\begin{aligned} I(\alpha, \beta, \gamma; n_\ell(Vr_{32})) &= \sqrt{\frac{2}{\pi}} \int_0^{+\infty} \int_0^{+\infty} \int_{|r_{32}-r_{31}|}^{r_{32}+r_{31}} r_{32}^{\frac{1}{2}-1} N_{\ell+\frac{1}{2}}(Vr_{32}) \exp(-\alpha r_{32} - \beta r_{31} - \gamma r_{21}) \\ dr_{32} dr_{31} dr_{21} &= \sqrt{\frac{2}{\pi}} \frac{2}{\beta^2 - \gamma^2} \left\{ \int_0^{+\infty} r_{32}^{\frac{1}{2}-1} N_{\ell+\frac{1}{2}}(Vr_{32}) \exp[-(\alpha + \beta)r_{32}] dr_{32} \right. \\ &\quad \left. - \int_0^{+\infty} r_{32}^{\frac{1}{2}-1} N_{\ell+\frac{1}{2}}(Vr_{32}) \exp[-(\alpha + \gamma)r_{32}] dr_{32} \right\} \\ &= \sqrt{\frac{2}{\pi}} \frac{2}{\beta^2 - \gamma^2} [G(\alpha + \beta, V) - G(\alpha + \gamma, V)] \end{aligned} \quad (12)$$

where the  $g$ -function is

$$\begin{aligned} G(\alpha + \beta, V) &= \int_0^{+\infty} r_{32}^{\frac{1}{2}-1} N_{\ell+\frac{1}{2}}(Vr_{32}) \exp[-(\alpha + \beta)r_{32}] dr_{32} \\ &= -\frac{2}{\pi} \frac{\ell!}{[(\alpha + \beta)^2 + V^2]^{\frac{1}{4}}} \cdot Q_{-\frac{1}{2}}^{-\ell-\frac{1}{2}}\left(\frac{\alpha + \beta}{\sqrt{[(\alpha + \beta)^2 + V^2]}}\right) \end{aligned} \quad (13)$$

where  $Q_\nu^\mu$  are the associated Legendre functions of the second kind. The explicit expression of the  $G(\alpha + \beta, V)$  in terms of hypergeometric functions is extremely cumbersome (see, e.g., the formula on page 733 in [3]) and it is not presented here.

### III. FORMULAS FOR THE PARTIAL DERIVATIVES

As we mentioned above the formulas presented above for the  $J(\alpha, \beta, \gamma; j_\ell(Vr_{32}))$  and  $I(\alpha, \beta, \gamma; n_\ell(Vr_{32}))$  integrals are not the final formulas which can directly be used in calculations. In actual calculations one needs to determine the third order derivatives from these integrals (see, Eq.(3)) in respect with the three parameters  $\alpha, \beta, \gamma$ . Only after this procedure

we find the values which are the final expressions for three-body integrals arising in actual applications. Analytical computation of the partial derivative of the  $J(\alpha, \beta, \gamma; j_\ell(Vr_{32}))$  and  $I(\alpha, \beta, \gamma; n_\ell(Vr_{32}))$  in respect with the parameter  $\alpha$  is straightforward. For simplicity below, we restrict ourselves to the analysis of the  $J$ -integral integral only. Note that Eq.(9) can also be written in the form

$$\begin{aligned} F(\alpha + \beta, V) &= \frac{\ell!}{2^\ell \sqrt{2V} \Gamma(\ell + \frac{3}{2})} \cdot (q^2)^{\frac{\ell+1}{2}} \cdot {}_2F_1\left(\frac{\ell+1}{2}, \frac{\ell+1}{2}; \ell + \frac{3}{2}; q^2\right) \\ &= A(\ell, V) \cdot (q^2)^{\frac{\ell+1}{2}} \cdot {}_2F_1\left(\frac{\ell+1}{2}, \frac{\ell+1}{2}; \ell + \frac{3}{2}; q^2\right) \end{aligned} \quad (14)$$

where  $A(\ell, V) = \frac{\ell!}{2^\ell \sqrt{2V} \Gamma(\ell + \frac{3}{2})}$  is a  $q$ -independent function. The partial derivative in respect with the parameter  $\alpha$  is determined with the use of the following relation

$$\frac{\partial f}{\partial \alpha} = \frac{2q^4}{V^2}(\alpha + \beta) \frac{\partial f}{\partial q^2} = \frac{\partial f}{\partial \beta} \quad (15)$$

where the function  $f = f(\alpha + \beta)$ . Analogously, for the functions which depend upon the sum  $\alpha + \gamma$  the partial derivative is

$$\frac{\partial f_1}{\partial \alpha} = \frac{2q^4}{V^2}(\alpha + \gamma) \frac{\partial f_1}{\partial q^2} = \frac{\partial f_1}{\partial \gamma} \quad (16)$$

where the function  $f_1 = f_1(\alpha + \gamma)$  depends upon the sum of the two parameters  $\alpha$  and  $\gamma$ .

Let us apply these formulas to the  $F(\alpha + \beta, V)$  function defined in Eq.(14). For the partial derivative of the  $F(\alpha + \beta, V)$  function in respect to the  $\alpha$  one finds

$$\begin{aligned} \frac{\partial F}{\partial \alpha} &= 2(\alpha + \beta)V^2 A(\ell, V) \left\{ (q^2)^{\frac{\ell+1}{2}} \cdot {}_2F_1\left(\frac{\ell+1}{2}, \frac{\ell+1}{2}; \ell + \frac{3}{2}; q^2\right) + (q^2)^{\frac{\ell+3}{2}} \cdot \frac{(\ell+1)^2}{2(2\ell+3)} \right. \\ &\quad \left. {}_2F_1\left(\frac{\ell+3}{2}, \frac{\ell+3}{2}; \ell + \frac{5}{2}; q^2\right) \right\} = \frac{\partial F}{\partial \beta} \end{aligned} \quad (17)$$

where we have used the formula

$$\frac{d {}_2F_1(a, b; c; z)}{dz} = \frac{ab}{c} \cdot {}_2F_1(a+1, b+1; c+1; z) \quad (18)$$

known from the theory of hypergeometric functions (see, e.g., [4]). Analogous formula for the  $F(\alpha + \gamma, V)$  takes the form

$$\begin{aligned} \frac{\partial F}{\partial \alpha} &= 2(\alpha + \gamma)V^2 A(\ell, V) \left\{ (q^2)^{\frac{\ell+1}{2}} \cdot {}_2F_1\left(\frac{\ell+1}{2}, \frac{\ell+1}{2}; \ell + \frac{3}{2}; q^2\right) + (q^2)^{\frac{\ell+3}{2}} \cdot \frac{(\ell+1)^2}{2(2\ell+3)} \right. \\ &\quad \left. {}_2F_1\left(\frac{\ell+3}{2}, \frac{\ell+3}{2}; \ell + \frac{5}{2}; q^2\right) \right\} = \frac{\partial F}{\partial \gamma} \end{aligned} \quad (19)$$

Note that the partial derivative of the functions  $F(\alpha + \beta, V)$  and  $F(\alpha + \gamma, V)$ , Eq.(14), upon the parameters  $\alpha, \beta$  and/or  $\gamma$  is always written in the form of a product of the power-type function of  $q^2$  and the hypergeometric function  ${}_2F_1$  which also depend upon the variable  $q^2$ . This simplifies analytical (and numerical) computation of the three-particle integrals with spherical Bessel and Neumann functions.

#### IV. CONCLUSION

We have developed an alternative approach to produce the closed analytical formulas for the three-particles integrals which include spherical Bessel functions of the first and second kind. In contrast with our approach described in [1] this method is based on the use of the general analytical formula, Eqs.(4) - (5), for three-body integrals written in the relative coordinates  $r_{32}, r_{31}$  and  $r_{21}$ . In a number of actual applications this (new) approach has a number of obvious advantages. However, in some special cases our old approach is much simpler and directly leads to the final (analytical and/or numerical) answer.

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